

# Package ‘MSstatsResponse’

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**Type** Package

**Title** Statistical Methods for Chemoproteomics Dose-Response Analysis

**Version** 1.1.0

**Description** Tools for detecting drug-protein interactions and estimating IC50 values from chemoproteomics data. Implements semi-parametric isotonic regression, bootstrapping, and curve fitting to evaluate compound effects on protein abundance.

**URL** <https://github.com/Vitek-Lab/MSstatsResponse>

**BugReports** <https://github.com/Vitek-Lab/MSstatsResponse/issues>

**License** Artistic-2.0

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---

.extractTemplatesFromData

*Helper function to extract template profiles from user data*

---

### Description

Helper function to extract template profiles from user data

### Usage

```
.extractTemplatesFromData(
  data,
  strong_proteins,
  weak_proteins,
  no_interaction_proteins,
  drug_name,
  concentrations
)
```

### Arguments

data	Prepared dose-response data
strong_proteins	Vector of protein IDs for strong responders
weak_proteins	Vector of protein IDs for weak responders
no_interaction_proteins	Vector of protein IDs for non-responders
drug_name	Drug to extract templates for
concentrations	Concentrations to include in template (in nM)

**Value**

List with template data for each interaction type

---

bootstrapIC50	<i>Bootstrap IC50 Estimates and Confidence Interval (ratio scale)</i>
---------------	-----------------------------------------------------------------------

---

**Description**

Bootstrap IC50 Estimates and Confidence Interval (ratio scale)

**Usage**

```
bootstrapIC50(
  dose,
  response,
  n_samples = 1000,
  alpha = 0.1,
  increasing = FALSE,
  target_response = 0.5,
  transform_x = TRUE
)
```

**Arguments**

dose	Numeric vector of dose values.
response	Numeric vector of response values (on log2 scale).
n_samples	Number of bootstrap samples (default = 1000).
alpha	Significance level for confidence interval (default = 0.10).
increasing	Logical. Fit non-decreasing if TRUE.
target_response	Numeric value for response level (default = 0.5).
transform_x	Logical. If TRUE, applies log10(dose + 1) transformation. Default = TRUE.

**Value**

List with mean IC50, CI bounds, and transformed estimates.

---

bootstrapIC50LogScale *Bootstrap IC50 Estimates and Confidence Interval (log scale)*

---

**Description**

Bootstrap IC50 Estimates and Confidence Interval (log scale)

**Usage**

```
bootstrapIC50LogScale(
  x,
  y,
  n_samples = 1000,
  alpha = 0.05,
  increasing = FALSE,
  target_response = 0.5
)
```

**Arguments**

x	Numeric vector of dose values.
y	Numeric vector of log2 response values.
n_samples	Number of bootstrap samples (default = 1000).
alpha	Significance level for confidence interval (default = 0.05).
increasing	Logical. Fit non-decreasing if TRUE.
target_response	Numeric value for response level (default = 0.5).

**Value**

List with mean IC50, CI bounds, and transformed estimates.

---

convertGroupToNumericDose  
*Convert MSstats GROUP labels to numeric dose in nM and extract drug name*

---

**Description**

Convert MSstats GROUP labels to numeric dose in nM and extract drug name

**Usage**

```
convertGroupToNumericDose(group_vector)
```

**Arguments**

group_vector	A character or factor vector with GROUP labels (e.g., "Dasatinib_003uM")
--------------	--------------------------------------------------------------------------

**Value**

A data frame with two columns: dose\_nM (numeric), and drug (character).

**Examples**

```
# Example 1: Basic conversion with mixed units
groups <- c("DMSO", "Dasatinib_001uM", "Dasatinib_010uM",
           "Dasatinib_100nM", "Dasatinib_1000nM")
dose_info <- convertGroupToNumericDose(groups)
print(dose_info)

# Example 2: Handle multiple drugs
multi_drug_groups <- c("DMSO",
                     "Dasatinib_001uM", "Dasatinib_010uM",
                     "Imatinib_001uM", "Imatinib_010uM")
multi_dose_info <- convertGroupToNumericDose(multi_drug_groups)
print(multi_dose_info)

# Show unique drugs found
print(unique(multi_dose_info$drug))
```

---

DIA\_MSstats\_Normalized

*Example pre-processed DIA-MS dataset*

---

**Description**

This dataset contains normalized protein-level data from a DIA-MS chemoproteomics experiment, pre-processed using MSstats.

**Usage**

```
DIA_MSstats_Normalized
```

**Format**

A data frame with protein-level abundance values and associated MSstats metadata column names.

**Details**

It is used in the MSstatsResponse vignette to demonstrate data formatting and downstream dose-response analysis.

The dataset is formatted using the standard MSstats preprocessing workflow. For more information on preprocessing mass spectrometry-based proteomics experiments, see the vignettes for MSstats and/or MSstatsTMT.

Below is an example of how such data can be prepared:

```
# Read raw data (example with Spectronaut output)
raw_data <- readr::read_tsv("path/to/spectronaut_report.tsv")

# Convert to MSstats format
```

```

msstats_data <- MSstats::SpectronauttoMSstatsFormat(raw_data)

# Process data: normalization and protein summarization
processed_data <- MSstats::dataProcess(
  msstats_data,
  normalization = "equalizeMedians", # or FALSE for no normalization
  summaryMethod = "TMP",             # Tukey's median polish
  MBimpute = TRUE,                   # Impute missing values
  maxQuantileforCensored = 0.999
)

```

### Examples

```

data("DIA_MSstats_Normalized")
head(DIA_MSstats_Normalized)

```

---

doseResponseFit	<i>Drug-protein interaction detection tested by F-test (fitted curve vs average response)</i>
-----------------	-----------------------------------------------------------------------------------------------

---

### Description

Fits an isotonic regression model to protein abundance data. Performs an F-test to assess the significance of the dose-response curve and applies FDR correction.

### Usage

```

doseResponseFit(
  data,
  weights = NULL,
  increasing = FALSE,
  transform_dose = TRUE,
  ratio_response = FALSE
)

```

### Arguments

data	Protein-level data, formatted with MSstatsPreparedoseResponseFit().
weights	Optional numeric vector of weights. Defaults to equal weights.
increasing	Logical. If TRUE, fits a non-decreasing model. If FALSE, fits non-increasing.
transform_dose	Logical. If TRUE, applies log <sub>10</sub> (dose + 1) transformation. Default is TRUE.
ratio_response	Logical. If TRUE, converts log <sub>2</sub> abundance to ratios relative to DMSO. Default is FALSE.

### Value

A data frame with protein-wise F-test results and BH-adjusted p-values.

**Examples**

```
# Load example data
data_path <- system.file("extdata", "DIA_MSstats_Normalized.RDS",
                        package = "MSstatsResponse")
dia_data <- readRDS(data_path)

# Convert GROUP to dose
dose_info <- convertGroupToNumericDose(dia_data$ProteinLevelData$GROUP)
dia_data$ProteinLevelData$dose <- dose_info$dose_nM * 1e-9
dia_data$ProteinLevelData$drug <- dose_info$drug

# Prepare data for analysis
prepared_data <- MSstatsPrepareDoseResponseFit(
  dia_data$ProteinLevelData,
  dose_column = "dose",
  drug_column = "drug",
  protein_column = "Protein",
  log_abundance_column = "LogIntensities"
)

# Subset for quick example
example_data <- prepared_data[prepared_data$protein %in%
                             unique(prepared_data$protein)[1:5], ]

# Example 1: Basic interaction detection on log2 scale
interaction_results <- doseResponseFit(
  data = example_data,
  increasing = FALSE,
  transform_dose = TRUE,
  ratio_response = FALSE
)

# View results
print(interaction_results)

# Check significant interactions
significant <- interaction_results[interaction_results$adjust_pval < 0.05, ]
print(paste("Found", nrow(significant), "significant interactions"))

## Not run:
# Example 2: Full dataset analysis
full_results <- doseResponseFit(
  data = prepared_data,
  increasing = FALSE,
  transform_dose = TRUE,
  ratio_response = FALSE
)

## End(Not run)
```

**Description**

Fits an isotonic regression model to protein intensity data with log-transformed drug doses. Optionally performs an F-test to assess the significance of the dose-response curve.

**Usage**

```
fitIsotonicRegression(
  x,
  y,
  w = rep(1, length(y)),
  increasing = FALSE,
  transform_x = TRUE,
  ratio_y = FALSE,
  test_significance = FALSE
)
```

**Arguments**

x	Numeric vector of dose values.
y	Numeric vector of response values.
w	Optional numeric vector of weights. Defaults to equal weights.
increasing	Logical. If TRUE, fits a non-decreasing model. If FALSE, fits non-increasing.
transform_x	Logical. If TRUE, applies $\log_{10}(x + 1)$ transformation. Default is TRUE.
ratio_y	Logical. If TRUE, converts $\log_2$ abundance to ratios relative to DMSO. Default is FALSE.
test_significance	Logical. If TRUE, performs F-test to assess significance.

**Value**

A list representing the isotonic regression model (class = "isotonic\_model").

---

futureExperimentSimulation

*Test future experimental design using simulated data with user-defined or default templates*

---

**Description**

Test future experimental design using simulated data with user-defined or default templates

**Usage**

```
futureExperimentSimulation(
  N_proteins = 300,
  N_rep = 3,
  N_Control_Rep = NULL,
  Concentrations = c(0, 1, 3, 10, 30, 100, 300, 1000, 3000),
  IC50_Prediction = FALSE,
```

```

    data = NULL,
    strong_proteins = NULL,
    weak_proteins = NULL,
    no_interaction_proteins = NULL,
    drug_name = NULL
  )

```

### Arguments

<code>N_proteins</code>	Number of proteins to simulate. Default = 300.
<code>N_rep</code>	Number of replicates for each drug concentration. Default = 3.
<code>N_Control_Rep</code>	Number of control replicates. If NULL, uses <code>N_rep</code> .
<code>Concentrations</code>	Numeric vector of drug concentrations (in nM scale). Default = <code>c(0, 1, 3, 10, 30, 100, 300, 1000, 3000)</code> .
<code>IC50_Prediction</code>	Logical. If TRUE, perform IC50 prediction. Default = FALSE.
<code>data</code>	Optional. User's prepared dose-response data (e.g., from <code>MSstatsPrepareDoseResponseFit</code> ). If provided, will extract templates from this data instead of using defaults.
<code>strong_proteins</code>	Character vector of protein IDs to use as strong interaction templates. Only used if data is provided.
<code>weak_proteins</code>	Character vector of protein IDs to use as weak interaction templates. Only used if data is provided.
<code>no_interaction_proteins</code>	Character vector of protein IDs to use as no interaction templates. Only used if data is provided.
<code>drug_name</code>	Character. Name of drug to extract templates for. Default = first non-DMSO drug in data.

### Value

A list containing simulated data, MSstats formatted data, dose-response fit results, hit rate plots, and optionally IC50 predictions.

### Examples

```

# Example 1: Quick simulation with default templates (small scale for speed)
sim_results <- futureExperimentSimulation(
  N_proteins = 50, # Small number for quick example
  N_rep = 2,
  N_Control_Rep = 3,
  Concentrations = c(0, 10, 100, 1000), # Fewer doses for speed
  IC50_Prediction = FALSE
)

# View hit rates
print(sim_results$Hit_Rates_Data)

# Check simulation results
print(paste("Simulated", nrow(sim_results$Simulated_Data), "data points"))

```

```

## Not run:
# Example 2: Full simulation with standard parameters
full_sim <- futureExperimentSimulation(
  N_proteins = 3000,
  N_rep = 3,
  N_Control_Rep = 6,
  Concentrations = c(0, 1, 3, 10, 30, 100, 300, 1000, 3000),
  IC50_Prediction = TRUE
)

# Display power analysis plot
print(full_sim$Hit_Rates_Plot)

# Example 3: Using custom templates from your own data
# Load and prepare your data
data_path <- system.file("extdata", "DIA_MSstats_Normalized.RDS",
  package = "MSstatsResponse")
dia_data <- readRDS(data_path)

dose_info <- convertGroupToNumericDose(dia_data$ProteinLevelData$GROUP)
dia_data$ProteinLevelData$dose <- dose_info$dose_nM * 1e-9
dia_data$ProteinLevelData$drug <- dose_info$drug

prepared_data <- MSstatsPrepareDoseResponseFit(
  dia_data$ProteinLevelData,
  dose_column = "dose",
  drug_column = "drug",
  protein_column = "Protein",
  log_abundance_column = "LogIntensities"
)

# Run simulation with custom templates
custom_sim <- futureExperimentSimulation(
  N_proteins = 1000,
  N_rep = 3,
  data = prepared_data,
  strong_proteins = c("PROTEIN_A"),
  weak_proteins = c("PROTEIN_B"),
  no_interaction_proteins = c("PROTEIN_C"),
  drug_name = "Drug1",
  Concentrations = c(0, 1, 10, 100, 1000, 3000)
)

## End(Not run)

```

---

MSstatsPrepareDoseResponseFit

*Prepare data for dose-response fitting with isotonic regression*

---

## Description

Prepare data for dose-response fitting with isotonic regression

**Usage**

```
MSstatsPrepareDoseResponseFit(
  data,
  dose_column = "dose",
  drug_column = "drug",
  protein_column = "Protein",
  log_abundance_column = "LogIntensities",
  transform_nM_to_M = NULL
)
```

**Arguments**

<code>data</code>	A data.frame (e.g. <code>data\$ProteinLevelData</code> from MSstats)
<code>dose_column</code>	Name of the column containing dose values (e.g., "dose")
<code>drug_column</code>	Name of column containing treatment name (e.g. drug name )
<code>protein_column</code>	Name of the column containing protein identifiers (e.g., "Protein")
<code>log_abundance_column</code>	Name of the column with log-transformed abundance values (e.g., "LogIntensities")
<code>transform_nM_to_M</code>	Logical. If TRUE, converts dose values from nanomolar (nM) to molar (M) by multiplying by $10^{-9}$ . Use when <code>dose_column</code> contains nM values but analysis requires M units. Default is NULL (no transformation applied).

**Value**

A standardized data.frame with columns: dose, response, protein

**Examples**

```
# Load example data
data_path <- system.file("extdata", "DIA_MSstats_Normalized.RDS",
  package = "MSstatsResponse")
dia_data <- readRDS(data_path)

# Example 1: Basic data preparation with dose already in M
# First add dose column if using GROUP labels
dose_info <- convertGroupToNumericDose(dia_data$ProteinLevelData$GROUP)
dia_data$ProteinLevelData$dose <- dose_info$dose_nM * 1e-9 # Convert to M
dia_data$ProteinLevelData$drug <- dose_info$drug

prepared_data <- MSstatsPrepareDoseResponseFit(
  data = dia_data$ProteinLevelData,
  dose_column = "dose",
  drug_column = "drug",
  protein_column = "Protein",
  log_abundance_column = "LogIntensities"
)

# Check structure
str(prepared_data)
head(prepared_data)
```

```

# Example 2: Convert dose from nM to M during preparation
dia_data$ProteinLevelData$dose_nM <- dose_info$dose_nM # Keep in nM

prepared_data_converted <- MSstatsPrepareDoseResponseFit(
  data = dia_data$ProteinLevelData,
  dose_column = "dose_nM",
  drug_column = "drug",
  protein_column = "Protein",
  log_abundance_column = "LogIntensities",
  transform_nM_to_M = TRUE # Convert nM to M
)

# Verify conversion
print(unique(prepared_data_converted$dose))

## Not run:
# Example 3: Working with custom column names
custom_data <- data.frame(
  ProteinID = rep(c("P1", "P2"), each = 10),
  Treatment = rep(c("DMSO", "Drug1"), 10),
  Concentration = rep(c(0, 1, 10, 100, 1000), 4),
  Log2Abundance = rnorm(20, mean = 20, sd = 1)
)

prepared_custom <- MSstatsPrepareDoseResponseFit(
  data = custom_data,
  dose_column = "Concentration",
  drug_column = "Treatment",
  protein_column = "ProteinID",
  log_abundance_column = "Log2Abundance",
  transform_nM_to_M = TRUE
)

## End(Not run)

```

---

plotHitRateMSstatsResponse

*Plot hit rates by category*

---

### Description

Plot hit rates by category

### Usage

```
plotHitRateMSstatsResponse(results, rep_count, concentration_count)
```

### Arguments

results	Output of interaction test from doseResponseFit()
rep_count	Number of replicates per concentration in simulation
concentration_count	Number of concentrations in simulation

**Value**

A list containing the plot and plot data

---

plotIsotonic	<i>Plot Isotonic Regression Model</i>
--------------	---------------------------------------

---

**Description**

Plot Isotonic Regression Model

**Usage**

```
plotIsotonic(
  fit,
  ratio = TRUE,
  show_ic50 = FALSE,
  drug_name = NULL,
  protein_name = NULL,
  x_lab = expression(Log[10] ~ "[drug (M)]"),
  y_lab = "Log2 Intensity",
  title = NULL,
  ci = NULL,
  legend = FALSE,
  theme_style = "classic",
  original_label = FALSE
)
```

**Arguments**

fit	A model object returned by fitIsotonicRegression().
ratio	Logical. If TRUE, shows plot on the ratio scale relative to DMSO (i.e. 0-1 scale). Default is FALSE.
show_ic50	Logical. If TRUE, adds vertical line and annotation for IC50.
drug_name	Drug name for plotting data.
protein_name	Protein name for plot.
x_lab	Label for x-axis.
y_lab	Label for y-axis.
title	Title for the plot.
ci	Logical. Include IC50 95% confidence interval bands if TRUE. Default is FALSE.
legend	Logical. Show legend if TRUE.
theme_style	ggplot2 theme name to apply (default = "classic").
original_label	Logical. If TRUE, replace x-axis tick labels with original dose labels.

**Value**

A ggplot object.

---

predictIC50	<i>Predict IC50 (dose where response = target) for each protein and drug</i>
-------------	------------------------------------------------------------------------------

---

### Description

Predict IC50 (dose where response = target) for each protein and drug

### Usage

```
predictIC50(
  data,
  n_samples = 1000,
  alpha = 0.1,
  increasing = FALSE,
  transform_dose = TRUE,
  ratio_response = TRUE,
  bootstrap = TRUE,
  BPPARAM = bpparam(),
  target_response = 0.5
)
```

### Arguments

<code>data</code>	A data frame with columns: protein, drug, dose, response.
<code>n_samples</code>	Number of bootstrap samples. Default = 1000.
<code>alpha</code>	Confidence level. Default = 0.10.
<code>increasing</code>	Logical. If TRUE, fit a non-decreasing trend. Default = FALSE.
<code>transform_dose</code>	Logical. If TRUE, applies $\log_{10}(\text{dose} + 1)$ transformation. Default = TRUE.
<code>ratio_response</code>	Logical. If TRUE, use ratio response; else use $\log_2$ scale. Default = TRUE.
<code>bootstrap</code>	Logical. If FALSE, skip confidence interval bootstrap estimation and only return IC50. Default = TRUE.
<code>BPPARAM</code>	A <code>BiocParallelParam</code> for parallel processing. The recommended usage is to <i>register</i> a backend once (e.g., <code>register(MulticoreParam(workers=4))</code> on Linux/macOS or <code>register(SnowParam(workers=4, type="SOCK"))</code> on Windows) and pass <code>BPPARAM = bpparam()</code> . Default <code>bpparam()</code> .
<code>target_response</code>	Numeric, the response fraction (e.g., 0.5, 0.25, 0.75). Default = 0.5.

### Value

A data frame with columns: protein, drug, IC50, IC50\_lower\_bound, IC50\_upper\_bound.

### Examples

```
# Load example data
data_path <- system.file("extdata", "DIA_MSstats_Normalized.RDS",
                        package = "MSstatsResponse")
dia_data <- readRDS(data_path)
```

```
# Convert GROUP to dose
dose_info <- convertGroupToNumericDose(dia_data$ProteinLevelData$GROUP)
dia_data$ProteinLevelData$dose <- dose_info$dose_nM * 1e-9
dia_data$ProteinLevelData$drug <- dose_info$drug

# Prepare data for analysis
prepared_data <- MSstatsPrepareDoseResponseFit(
  dia_data$ProteinLevelData,
  dose_column = "dose",
  drug_column = "drug",
  protein_column = "Protein",
  log_abundance_column = "LogIntensities"
)

# Subset to fewer proteins for example
example_data <- prepared_data[prepared_data$protein %in%
  unique(prepared_data$protein)[1:3], ]

# Example 1: Quick IC50 estimation without bootstrap (fast)
ic50_quick <- predictIC50(
  data = example_data,
  bootstrap = FALSE
)
print(ic50_quick)

## Not run:
# Example 2: Full IC50 estimation with bootstrap confidence intervals
ic50_results <- predictIC50(
  data = prepared_data,
  n_samples = 1000,
  alpha = 0.10,
  ratio_response = TRUE,
  bootstrap = TRUE
)

# Example 3: Parallel processing for large datasets
library(BiocParallel)
ic50_parallel <- predictIC50(
  data = prepared_data,
  n_samples = 1000,
  BPPARAM = bpparam(),
  bootstrap = TRUE
)

# Example 4: IC50 at different response levels (IC25, IC75)
ic25_results <- predictIC50(
  data = prepared_data,
  target_response = 0.25,
  bootstrap = TRUE
)

## End(Not run)
```

---

predictIC50Parallel *Parallel version of predictIC50 function*

---

### Description

Runs predictIC50 on the entire dataset in parallel across proteins.

### Usage

```
predictIC50Parallel(
  data,
  n_samples = 1000,
  alpha = 0.1,
  increasing = FALSE,
  transform_dose = TRUE,
  ratio_response = TRUE,
  bootstrap = TRUE,
  numberOfCores = 2
)
```

### Arguments

data	A data frame with columns: protein, drug, dose, response.
n_samples	Number of bootstrap samples. Default = 1000.
alpha	Confidence level. Default = 0.10.
increasing	Logical. If TRUE, fit non-decreasing trend. Default = FALSE.
transform_dose	Logical. If TRUE, applies log10(dose + 1) transformation. Default = TRUE.
ratio_response	Logical. If TRUE, use ratio response; else use log2 scale. Default = TRUE.
bootstrap	Logical. If TRUE, compute bootstrap CIs. Default = TRUE.
numberOfCores	Number of cores for parallel processing. Default = 2.

### Value

A data frame with columns: protein, drug, IC50, lower CI, upper CI.

### Examples

```
# Load example data
data_path <- system.file("extdata", "DIA_MSstats_Normalized.RDS",
                        package = "MSstatsResponse")
dia_data <- readRDS(data_path)

# Convert GROUP to dose
dose_info <- convertGroupToNumericDose(dia_data$ProteinLevelData$GROUP)
dia_data$ProteinLevelData$dose <- dose_info$dose_nM * 1e-9
dia_data$ProteinLevelData$drug <- dose_info$drug

# Prepare data for analysis
prepared_data <- MSstatsPrepareDoseResponseFit(
  dia_data$ProteinLevelData,
```

```

    dose_column = "dose",
    drug_column = "drug",
    protein_column = "Protein",
    log_abundance_column = "LogIntensities"
  )

  # Subset for quick example
  example_data <- prepared_data[prepared_data$protein %in%
    unique(prepared_data$protein)[1:5], ]

  # Example 1: Quick parallel IC50 without bootstrap (2 cores)
  ic50_quick_parallel <- predictIC50Parallel(
    data = example_data,
    bootstrap = FALSE,
    numberOfCores = 2
  )
  print(ic50_quick_parallel)

```

---

```
simulateChemoProteinLevelNonParametric
```

*Simulate chemoproteomics data at the protein level - non-parametric approach*

---

## Description

Simulate chemoproteomics data at the protein level - non-parametric approach

## Usage

```

simulateChemoProteinLevelNonParametric(
  N_proteins = 3000,
  TP = 0.333,
  TW = 0.333,
  TN = 0.333,
  concentrations = c(0, 1, 3, 10, 30, 100, 300, 1000, 3000),
  rep = 3,
  seed = NULL,
  var_tech = 0.4,
  control_rep = NULL,
  template = list(strong_interaction = data.frame(dose = c(), LogIntensities = c()),
    weak_interaction = data.frame(dose = c(), LogIntensities = c()), no_interaction =
    data.frame(dose = c(), LogIntensities = c())),
  outlier_prob = 0.05
)

```

## Arguments

N_proteins	Number of proteins in simulation. Default = 3000.
TP	Proportion of strong interacting proteins. Default = 0.333.
TW	Proportion of weak interacting proteins. Default = 0.333.
TN	Proportion of non-interacting proteins. Default = 0.333.

concentrations	Numeric vector of drug concentrations in simulation experiment. Default = c(0, 1, 3, 10, 30, 100, 300, 1000, 3000).
rep	Number of replicates for each drug concentration. Default = 3.
seed	Simulation seed for reproducibility. Default = 3.
var_tech	Combined technical and biological variation. Default = 0.4.
control_rep	Number of control replicates. If NULL, uses rep.
template	List containing real protein level data representing different levels of interactions.
outlier_prob	Probability of sample outlier. Default = 0.05.

**Value**

A data.frame with simulated chemoproteomics data.

---

```
visualizeResponseProtein
```

*Plot isotonic regression fit with optional IC50 for a single protein and drug*

---

**Description**

Plot isotonic regression fit with optional IC50 for a single protein and drug

**Usage**

```
visualizeResponseProtein(
  data,
  protein_name,
  drug_name,
  ratio_response = TRUE,
  transform_dose = TRUE,
  show_ic50 = TRUE,
  add_ci = FALSE,
  n_samples = 1000,
  alpha = 0.1,
  increasing = FALSE,
  y_lab = "Ratio Response"
)
```

**Arguments**

data	Protein-level dataset (e.g., output of MSstatsPrepareDoseResponseFit).
protein_name	Character. Protein name to plot.
drug_name	Character. Drug name to plot.
ratio_response	Logical. If TRUE, compute IC50 on ratio scale; if FALSE, use log2 intensities.
transform_dose	Logical. If TRUE, applies log10(dose + 1). Default is TRUE.
show_ic50	Logical. If TRUE, adds vertical line and annotation for IC50.
add_ci	Logical. Include IC50 95% confidence interval bands if TRUE. Default is FALSE.

n_samples	Number of bootstrap samples if including confidence intervals. Default is 1000.
alpha	Alpha level for confidence intervals. Default is 0.05.
increasing	Logical. If TRUE, fits a non-decreasing model. If FALSE, fits non-increasing.
y_lab	Character. Label for the y-axis. Default is "Ratio Response".

**Value**

A ggplot object.

**Examples**

```
# Load example data
data_path <- system.file("extdata", "DIA_MSstats_Normalized.RDS",
                        package = "MSstatsResponse")
dia_data <- readRDS(data_path)

# Convert GROUP to dose
dose_info <- convertGroupToNumericDose(dia_data$ProteinLevelData$GROUP)
dia_data$ProteinLevelData$dose <- dose_info$dose_nM * 1e-9
dia_data$ProteinLevelData$drug <- dose_info$drug

# Prepare data for analysis
prepared_data <- MSstatsPrepareDoseResponseFit(
  dia_data$ProteinLevelData,
  dose_column = "dose",
  drug_column = "drug",
  protein_column = "Protein",
  log_abundance_column = "LogIntensities"
)

# Example 1: Basic dose-response visualization
plot1 <- visualizeResponseProtein(
  data = prepared_data,
  protein_name = "PROTEIN_A",
  drug_name = "Drug1",
  ratio_response = TRUE,
  show_ic50 = FALSE,
  add_ci = FALSE
)
print(plot1)

# Example 2: Add IC50 annotation
plot2 <- visualizeResponseProtein(
  data = prepared_data,
  protein_name = "PROTEIN_A",
  drug_name = "Drug1",
  ratio_response = TRUE,
  show_ic50 = TRUE,
  add_ci = FALSE
)
print(plot2)
```

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